2,2-Dimethylocta-3,4-dienal

Other names: 3,4-Octadienal, 2,2-dimethyl
2,2-Dimethyl-3,4-octadienal
Inchi: InChI=1S/C10H16O/c1-4-5-6-7-8-10(2,3)9-11/h6,8-9H,4-5H2,1-3H3
InchiKey: VSFHYKIILWBKOH-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CCCC=C=CC(C)(C)C=O
Mol. weight [g/mol]: 152.23
CAS: 590-71-6

Physical Properties

Property code	Value	Unit	Source
gf	145.14	kJ/mol	Joback Method
hf	-64.06	kJ/mol	Joback Method
hfus	18.86	kJ/mol	Joback Method
hvap	43.67	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.723		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinpol	1098.00		NIST Webbook
rinpol	1116.00		NIST Webbook
tb	481.06	K	Joback Method
tc	679.17	K	Joback Method
tf	248.31	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.27	J/mol×K	481.06	Joback Method
cpg	329.61	J/mol×K	514.08	Joback Method
cpg	343.15	J/mol×K	547.10	Joback Method
cpg	355.94	J/mol×K	580.12	Joback Method
cpg	368.01	J/mol×K	613.14	Joback Method

cpg	379.39	J/mol×K	646.15	Joback Method
cpg	390.13	J/mol×K	679.17	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C590716&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume